Perfluorotributylamine
311-89-7 | DTXSID0027141

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -47.8 °C

Global applicability domain: Outside

Local applicability domain index: 3.42e-01

Confidence level: 4.76e-01

Nearest Neighbors from the Training Set

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Perfluorotributylamine
Measured: -50.0
Predicted: -47.8

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1,1,1,2,2,3,3,4,4,5,5,6,6-
tridecafluoro-6-
[(tridecafluorohexyl)oxy]hexane
Measured: -90.0
Predicted: -77.0

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1-Propanamine, 1,1,2,2,3,3,3-
heptafluoro-N,N-
bis(heptafluoropropyl)-
Measured: -52.0
Predicted: -47.3

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Decane,
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-
heneicosafluoro-10-iodo-
Measured: 66.0
Predicted: 42.4

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Perfluorononane
Measured: -16.0
Predicted: -17.4